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Controlling the properties of nanomaterials -
Nucleation and growth of semiconductor, metal and
molecular nanoparticles

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In recent years, nanoscience and nanotechnology have played an ever increasing role in a large number of areas such as e.g. in information technology, in the telecommunications industry, in medicine and in materials science and engineering. Because of their size, intermediate between the dimensions of atoms and of bulk matter, nanoscale materials often exhibit unique properties. If one compares a crystal composed of only a few thousands of atoms to a bulk crystal, the fraction of the total number of atoms on the surface of the nanosized crystal is much larger than the corresponding fraction for the bulk solid. This results in a much higher chemical reactivity for the nanosized crystal and, in most cases, in a lower temperature of melting than for the bulk crystal. The unique properties of nanoscale materials have been the subject of intense research over the last decade and their enhanced efficiency, for instance when they are used as catalysts, has been demonstrated. One needs, however, to be able to control the properties of nanomaterials (size, shape and crystalline structure) to fully harness the powerful properties of these materials. In this talk, I will discuss how molecular simulation can help unravel the interplay between kinetics and thermodynamics during the formation of nanomaterials. In particular, I will examine how the control of the properties of the nanoparticles can be achieved during nucleation and growth. Examples of the formation of semiconductor, metal and molecular nanoparticles will be presented.